Hexachloro-1,3-butadiene
87-68-3 | DTXSID7020683

Model Performance

Model	Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.85	0.69	0.86	0.67	0.86	0.78

Model Results

Predicted value: 4.65

Global applicability domain: Outside

Local applicability domain index: 3.98e-01

Confidence level: 6.03e-01

Nearest Neighbors from the Training Set

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Hexachloro-1,3-butadiene
Measured: 4.78
Predicted: 4.65

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Hexachlorocyclopentadiene
Measured: 5.04
Predicted: 4.81

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Bis(trichloromethyl)sulfone
Measured: 3.30
Predicted: 3.49

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Tetrachloroethylene
Measured: 3.40
Predicted: 3.35

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Hexachloroethane
Measured: 4.14
Predicted: 4.00